Zeeman effect of the hyperfine structure levels in lithiumlike ions

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Abstract

The fully relativistic theory of the Zeeman splitting of the $(1s)^2 2s$ hyperfine-structure levels in lithiumlike ions with $Z = 6 - 32$ is considered for the magnetic field magnitude in the range from 1 to 10 T. The second-order corrections to the Breit – Rabi formula are calculated and discussed including the one-electron contributions as well as the interelectronic-interaction effects of order $1/Z$. The $1/Z$ corrections are evaluated within a rigorous QED approach. These corrections are combined with other interelectronic-interaction, QED, nuclear recoil, and nuclear size corrections to obtain high-precision theoretical values for the Zeeman splitting in Li-like ions with nonzero nuclear spin. The results can be used for a precise determination of nuclear magnetic moments from g-factor experiments.

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1   Introduction

Recent measurements of the g factor of hydrogenlike carbon and oxygen have reached an accuracy of about $2 \cdot 10^{-9}$ [1–3]. The experiments were performed on a single hydrogenlike ion confined in a Penning trap with a strong magnetic field ($B = 3.8$ T). These measurements considerably stimulated theoretical investigations of this effect [4–22]. Besides a new possibility for tests of the magnetic sector of quantum electrodynamics (QED), these investigations have already provided a new determination of the electron mass (see Refs. [3, 23] and references therein). Extensions of these experiments to systems with higher nuclear charge number Z and to ions with nonzero nuclear spin would also provide the basis for new determinations of the fine-structure constant [8, 24, 25], the nuclear magnetic moments [24], and the nuclear charge radii.

Extending theoretical description from an H-like to a Li-like ion, one encounters a serious complication due to the presence of additional electrons. A number of relativistic calculations of the g factor of Li-like ions were carried out previously [26–30]. However, to reach the accuracy comparable to the one for H-like ions, a systematic quantum electrodynamic (QED) treatment is required [16, 31–35].

For both H- and Li-like heavy ions with nonzero nuclear spin the ground-state Zeeman splitting caused by the magnetic field in the range from 1 to 10 T is much smaller than the hyperfine splitting and, therefore, the consideration can be conveniently reduced to the g factor value [19, 35]. However, for H-like ions with $Z = 1 - 20$, which are being under current experimental investigations at Mainz University, the Zeeman splitting is comparable with the hyperfine splitting if the magnitude of the homogeneous magnetic field does not exceed 10 T. This requires constructing the perturbation theory for degenerate states. To a good accuracy, the solution of the problem is given by the well-known Breit – Rabi formula [36–39]. The aforesaid experimental precision has, however, shown the need for an improvement of the Breit – Rabi formula for H-like ions [21].

In the present paper, we consider the Breit – Rabi formula for the $2s$ hyperfine-structure levels in lithiumlike ions. Evaluations of the coefficients of this formula should include corrections depending on the nuclear g factor. Besides a simple one-electron lowest-order nuclear-spin-dependent contribution, one should also calculate the second-order corrections caused by the hyperfine interaction and the interaction with the external magnetic field, taking into account the presence of the closed $(1s)^2$ electron shell. We perform such calculations in the range $Z = 6-32$, where the $2s$ HFS splitting can be comparable with the Zeeman splitting if the magnitude of the homogeneous magnetic field is in the range under consideration. The calculations are based on perturbation theory in the parameter $1/Z$ within a rigorous QED approach. The contributions of zeroth and first orders in $1/Z$ are taken into account for the magnetic-dipole correction and the contribution of zeroth order is taken into consideration for the electric-quadrupole correction. Also, the B^2-dependent correction is calculated, including the contributions of zeroth and first orders in $1/Z$. The obtained results are combined with other corrections to get accurate theoretical predictions for the Breit – Rabi formula coefficients for lithiumlike ions with nonzero nuclear spin. These predictions will be important for experimental investigations that are anticipated in the near future at University of Mainz and GSI [40].

Relativistic units ($\hbar = c = 1$) and the Heaviside charge unit ($\alpha = e^2/4\pi$, $e < 0$) are used in the paper. In some important cases, the final formulas contain $\hbar$ and c explicitly to be applicable for arbitrary system of units.

2 The Breit – Rabi formula in the lowest-order one-electron approximation

We consider a lithiumlike ion with nonzero nuclear spin I in a state of the valent electron with the total electron angular momentum $j = 1/2$. The ion is placed in a homogeneous magnetic field $\vec{B}$ directed along the z axis. The magnetic splitting is linear with respect to $\vec{B}$ only if one of the following conditions is fulfilled: either $\Delta E_{\mathrm{mag}} \ll \Delta E_{\mathrm{HFS}}$ or $\Delta E_{\mathrm{mag}} \gg \Delta E_{\mathrm{HFS}}$, where $\Delta E_{\mathrm{HFS}} = E(F+1) - E(F)$, $E(F) = E_{n\kappa} + \varepsilon_{\mathrm{hfs}}(F)$, $F = I \pm 1/2$ is the total atomic angular momentum, and $\varepsilon_{\mathrm{hfs}}(F)$ is the hyperfine-structure shift of the valent electron Dirac state with the one-electron energy in the Coulomb field of the nucleus

$$E_{n\kappa} = \frac{\gamma + n_r}{N} m_e \,. \tag{1}$$

Here n is the principal quantum number, $\kappa = (-1)^{j+l+\frac{1}{2}}(j + \frac{1}{2})$, $l = j \pm \frac{1}{2}$ defines the parity of the state, $n_r = n - |\kappa|$ is the radial quantum number, $\gamma = \sqrt{\kappa^2 - (\alpha Z)^2}$, $N = \sqrt{n_r^2 + 2n_r\gamma + \kappa^2}$, and m_e is the electron mass. It should be emphasized that in case the second inequality is fulfilled ΔE_{mag} must be much less than the distance to other Dirac's levels. In the intermediate $\vec{B}$ case, $\Delta E_{\mathrm{mag}} \sim \Delta E_{\mathrm{HFS}}$, we must take into account mixing the HFS sublevels with the same M_F, where $M_F = -F, -F+1, ..., F-1, F$ is the z projection of the total angular momentum. For the states with the total electron angular momentum $j = 1/2$, there are only two HFS levels $F = I - 1/2$ and $F' = I + 1/2$ with the same $M_F = -I + 1/2, ..., I - 1/2$. This greatly simplifies the theory. In what follows, we restrict our consideration to the ground state of the valent electron.

Denoting [1] $\Delta E_{\text{mag}} = E - \frac{E^{(2s)}(F) + E^{(2s)}(F+1)}{2}$, one can derive for the Zeeman splitting

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left[a_1 M_F x \pm \frac{1}{2} \sqrt{1 + \frac{4M_F}{2I+1} c_1 x + c_2 x^2} \right], \tag{2}$$

where $x = \mu_0 B / \Delta E_{\text{HFS}}^{(2s)}$, $\mu_0 = |e|\hbar/(2m_e c)$ is the Bohr magneton,

$$a_1 = -g_I', \tag{3}$$
$$c_1 = g_j + g_I', \tag{4}$$
$$c_2 = (g_j + g_I')^2, \tag{5}$$

g_j is the ground-state bound-electron g factor of the lithiumlike ion,

$$g_j = g_{\text{D}} + \Delta g_{\text{int}} + \Delta g_{\text{QED}} + \Delta g_{\text{rec}}^{(e)} + \Delta g_{\text{NS}} + \Delta g_{\text{NP}}, \tag{6}$$

g_{D} is the one-electron Dirac value for a point-charge nucleus,

$$g_{\text{D}} = \frac{2[\sqrt{2 + 2\gamma} + 1]}{3} = 2 - \frac{(\alpha Z)^2}{6} + \dots, \tag{7}$$

$\gamma = \sqrt{1 - (\alpha Z)^2}$, Δg_{int} is the interelectronic-interaction correction, Δg_{QED} is the QED correction, $\Delta g_{\text{rec}}^{(e)}$ is the nuclear recoil correction to the bound-electron g factor, Δg_{NS} is the nuclear size correction, Δg_{NP} is the nuclear polarization correction, g_I' is the nuclear g factor expressed in the Bohr magnetons,

$$g_I' = \frac{m_e}{m_p}(g_I + \Delta g_{\text{rec}}^{(n)}), \tag{8}$$

m_p is the proton mass, $g_I = \mu/(\mu_N I)$, $\mu = \langle II|\mu_z|II\rangle$ is the nuclear magnetic moment, μ_z is the z projection of the nuclear magnetic moment operator $\vec{\mu}$ acting in the space of nuclear wave functions $|IM_I\rangle$ with the total angular momentum I and its projection M_I, $\mu_N = |e|\hbar/(2m_p c)$ is the nuclear magneton, and $\Delta g_{\text{rec}}^{(n)}$ is the recoil correction to the bound-nucleus g factor (see section 5). Eq. (2) is usually called the Breit – Rabi formula (see, e.g., Refs. [21, 36–39]). It covers Zeeman splitting from weak ($x \ll 1$) to strong ($x \gg 1$) fields including the intermediate region. For $F' = I + \frac{1}{2}$ and $M_F = \pm(I + \frac{1}{2})$ the splitting is linear in the first order of perturbation theory under arbitrary magnetic induction,

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left[\frac{1}{2} \pm d_1 x \right], \tag{9}$$

where

$$d_1 = \frac{1}{2} g_j - I g_I' \tag{10}$$

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[1] In the present paper, the energy of a Zeeman sublevel ΔE_{mag} is counted with respect to the mean energy $\frac{E^{(2s)}(F) + E^{(2s)}(F')}{2}$ of the hyperfine structure doublet [38, 39]. To count the energy from the hyperfine centroid of the doublet [36, 37], one should use the relation

$$\Delta E_{\text{mag}}^{\text{hc}} = \Delta E_{\text{mag}} - \frac{\Delta E_{\text{HFS}}^{(2s)}}{2(2I+1)}.$$

and the "−" and "+" signs refer to $M_F = -(I + \frac{1}{2})$ and $M_F = I + \frac{1}{2}$, respectively.

For Li-like ions with $I = 1/2$, $F = 0$ and $F' = 1$ and, therefore, the two mixed sublevels have $M_F = 0$. In this case the Breit – Rabi formula takes the form

$$\Delta E_{\text{mag}}(x) = \pm \frac{\Delta E_{\text{HFS}}^{(2s)}}{2} \sqrt{1 + c_2 x^2}, \tag{11}$$

and for $M_F = \pm 1$ the effect is described by Eq. (9) with $d_1 = \frac{1}{2}(g_j - g_I')$.

If the magnetic field is strong, $\Delta E_{\text{mag}} \gg \Delta E_{\text{HFS}}^{(2s)}$, Eqs. (2), (9), and (11) convert into formulas for the anomalous Zeeman effect of the $2s$ state.

In case the energy-level shift (splitting) due to interaction with $\vec{B}$ is much smaller than the hyperfine-structure splitting, $\Delta E_{\text{mag}} \ll \Delta E_{\text{HFS}}^{(2s)}$, we can express the linear-dependent part of this shift in terms of the atomic g factor,

$$\Delta E_{\text{mag}} = \pm \frac{\Delta E_{\text{HFS}}^{(2s)}}{2} + g(F)\mu_0 B M_F, \tag{12}$$

where, to the lowest-order approximation (see, e.g., Ref. [38]),

$$g(F) = g_D Y_{\text{el}}(F) - \frac{m_e}{m_p} g_I Y_{\text{nuc}}^{(\mu)}(F), \tag{13}$$

$$Y_{\text{el}}(F) = \frac{F(F+1) + 3/4 - I(I+1)}{2F(F+1)} = \begin{cases} -\frac{1}{2I+1} & \text{for } F = I - \frac{1}{2} \\ \frac{1}{2I+1} & \text{for } F = I + \frac{1}{2} \end{cases}, \tag{14}$$

$$Y_{\text{nuc}}^{(\mu)}(F) = \frac{F(F+1) + I(I+1) - 3/4}{2F(F+1)} = \begin{cases} \frac{2(I+1)}{2I+1} & \text{for } F = I - \frac{1}{2} \\ \frac{2I}{2I+1} & \text{for } F = I + \frac{1}{2} \end{cases}. \tag{15}$$

The total one-electron $2s$ g-factor value of a Li-like ion with nonzero nuclear spin can be represented by

$$\begin{aligned}
g(F) &= (g_D + \Delta g_{\text{int}} + \Delta g_{\text{QED}} + \Delta g_{\text{rec}}^{(e)} + \Delta g_{\text{NS}} + \Delta g_{\text{NP}}) Y_{\text{el}}(F) \\
&\quad - \frac{m_e}{m_p}(g_I + \Delta g_{\text{rec}}^{(n)}) Y_{\text{nuc}}^{(\mu)}(F) + \delta g_{\text{HFS}}^{(2s)}(F),
\end{aligned} \tag{16}$$

where the HFS correction $\delta g_{\text{HFS}}^{(2s)}(F) = \delta g_{\text{HFS}(\mu)}^{(2s)}(F) + \delta g_{\text{HFS}(Q)}^{(2s)}(F)$ [35] is briefly discussed below.

3 Hyperfine-interaction corrections to the ground state g factor

Let us start our consideration of the HFS correction to the ground-state g factor of a Li-like ion with the one-electron approximation. In this approximation, the interaction of the ion with the magnetic field can be represented as

$$V_{\vec{B}} = V_{\vec{B}}^{(e)} + V_{\vec{B}}^{(n)}. \tag{17}$$

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Here $V_{\vec{B}}^{(e)}$ describes the interaction of the valent $2s$ electron with the homogeneous magnetic field,

$$V_{\vec{B}}^{(e)} = -e(\vec{\alpha} \cdot \vec{A}) = \frac{|e|}{2}(\vec{\alpha} \cdot [\vec{B} \times \vec{r}]), \tag{18}$$

where the vector $\vec{\alpha}$ incorporates the Dirac α matrices, and

$$V_{\vec{B}}^{(n)} = -(\vec{\mu} \cdot \vec{B}) \tag{19}$$

describes the interaction of the nuclear magnetic moment $\vec{\mu}$ with $\vec{B}$. The hyperfine-interaction operator is given by the sum

$$V_{\mathrm{HFS}} = V_{\mathrm{HFS}}^{(\mu)} + V_{\mathrm{HFS}}^{(Q)}, \tag{20}$$

where $V_{\mathrm{HFS}}^{(\mu)}$ and $V_{\mathrm{HFS}}^{(Q)}$ are the magnetic-dipole and electric-quadrupole hyperfine-interaction operators, respectively. In the point-dipole approximation,

$$V_{\mathrm{HFS}}^{(\mu)} = \frac{|e|}{4\pi} \frac{(\vec{\alpha} \cdot [\vec{\mu} \times \vec{r}])}{r^3}, \tag{21}$$

and, in the point-quadrupole approximation,

$$V_{\mathrm{HFS}}^{(Q)} = -\alpha \sum_{m=-2}^{m=2} Q_{2m} \eta_{2m}^*(\vec{n}). \tag{22}$$

Here $Q_{2m} = \sum_{i=1}^{Z} r_i^2 C_{2m}(\vec{n}_i)$ is the operator of the electric-quadrupole moment of the nucleus, $\eta_{2m} = C_{2m}(\vec{n})/r^3$ is an operator that acts on electron variables, $\vec{n} = \vec{r}/r$, $\vec{n}_i = \vec{r}_i/r_i$, $\vec{r}$ is the position vector of the electron, $\vec{r}_i$ is the position vector of the i-th proton in the nucleus, $C_{lm} = \sqrt{4\pi/(2l+1)}\, Y_{lm}$, and Y_{lm} is a spherical harmonic. It must be stressed that the electric-quadrupole interaction should be taken into account only for ions with $I > 1/2$.

An unperturbed atomic eigenstate that corresponds to given values of F and M_F is a linear combination of products of electron and nuclear wave functions,

$$|nljIFM_F\rangle = \sum_{m_j, M_I} C_{jm_jIM_I}^{FM_F} |nljm_j\rangle|IM_I\rangle. \tag{23}$$

Here $C_{jm_jIM_I}^{FM_F}$ are the Clebsch-Gordan coefficients, $|nljm_j\rangle$ are the unperturbed one-electron wave functions, which are four-component eigenvectors of the Dirac equation for the Coulomb field, with the total angular momentum j and its projection m_j.

In the one-electron approximation, the magnetic-dipole and electric-quadrupole hyperfine-interaction corrections to the ground-state g factor of the Li-like ion are given by

$$\delta g_{\mathrm{HFS}(\mu,Q)}^{\mathrm{one-el.}(2s)} = \frac{2}{\mu_0 B M_F} \sum_{m_j M_I} \sum_{m'_j M'_I} C_{\frac{1}{2}m_jIM_I}^{FM_F} C_{\frac{1}{2}m'_jIM'_I}^{FM_F} \langle IM_I| \sum_{n}^{(\epsilon_n \neq \epsilon_v)} \frac{\langle v|V_{\vec{B}}^{(e)}|n\rangle\langle n|V_{\mathrm{HFS}}^{(\mu,Q)}|v'\rangle}{\varepsilon_v - \varepsilon_n}|IM'_I\rangle, \tag{24}$$

where $|v\rangle = |20\frac{1}{2}m_j\rangle$ and $|v'\rangle = |20\frac{1}{2}m'_j\rangle$ are the $2s$ states of the valent electron with the angular momentum projections m_j and m'_j, respectively, $|n\rangle \equiv |nljm_j\rangle$, $\varepsilon_v = E_{2,-1}$, and $\varepsilon_n \equiv E_{n\kappa}$. The summation in (24) runs over discrete as well as continuum states. The corresponding diagrams are presented in Fig. 1.

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The total hyperfine-interaction correction to the ground-state g factor of the Li-like ion is given by

$$\delta g_{\text{HFS}}^{(2s)} = \delta g_{\text{HFS}(\mu)}^{(2s)} + \delta g_{\text{HFS}(Q)}^{(2s)} \tag{25}$$

with

$$\delta g_{\text{HFS}(\mu)}^{(2s)} = \alpha^2 Z \frac{1}{12} \frac{\mu}{\mu_N} \frac{m_e}{m_p} \frac{1}{I} Y_{\text{nuc}}^{(\mu)}(F)[S_2(\alpha Z) + \frac{1}{Z} B_\mu(\alpha Z) + \frac{1}{Z^2} C_\mu(\alpha Z) + \dots] \tag{26}$$

and

$$\delta g_{\text{HFS}(Q)}^{(2s)} = \alpha^4 Z^3 \frac{23}{2160} Q \left(\frac{m_e c}{\hbar}\right)^2 Y_{\text{nuc}}^{(Q)}(F)[T_2(\alpha Z) + \frac{1}{Z} B_Q(\alpha Z) + \frac{1}{Z^2} C_Q(\alpha Z) + \dots]. \tag{27}$$

Here the angular factor is

$$Y_{\text{nuc}}^{(Q)}(F) = \begin{cases} -\frac{(I+1)(2I+3)}{I(2I-1)(2I+1)} & \text{for } F = I - \frac{1}{2} \\ \frac{1}{2I+1} & \text{for } F = I + \frac{1}{2} \end{cases}, \tag{28}$$

and $Q = 2\langle II|Q_{20}|II\rangle$ is the electric-quadrupole moment of the nucleus. The functions

$$S_2(\alpha Z) = \frac{12}{\alpha^2 Z \frac{m_e}{m_p} g_I Y_{\text{nuc}}^{(\mu)}(F)} \delta g_{\text{HFS}(\mu)}^{\text{one-el.}(2s)} \tag{29}$$

and

$$T_2(\alpha Z) = \frac{2160}{23\alpha^4 Z^3 Q \left(\frac{m_e c}{\hbar}\right)^2 Y_{\text{nuc}}^{(Q)}(F)} \delta g_{\text{HFS}(Q)}^{\text{one-el.}(2s)} \tag{30}$$

determine the one-electron contributions, which are discussed in detail in Ref. [19]. For the point-charge nucleus, the functions $S_2(\alpha Z)$ and $T_2(\alpha Z)$ are [19, 35]

$$S_2(\alpha Z) = \frac{8}{3N} \left\{ \frac{1}{N+2} \left[N + \frac{10(N+1)}{3N} \right] + \frac{(\alpha Z)^2}{\gamma(\gamma+1)} \left[\frac{2(N+1)}{3 - 4(\alpha Z)^2} + 1 \right] - \frac{1}{\gamma} \right\}$$
$$= 1 + \frac{229}{144}(\alpha Z)^2 + \dots \tag{31}$$

and

$$T_2(\alpha Z) = \frac{192[(N+\gamma+1)\{18 + 24\gamma - 12N + 8\gamma N^2\} + 15(1+\gamma)]}{23\gamma N^3 [15 - 16(\alpha Z)^2](N+\gamma+1)^2}$$
$$= 1 + \frac{427}{276}(\alpha Z)^2 + \dots, \tag{32}$$

where $N = \sqrt{2(1+\gamma)}$.

The interelectronic-interaction correction $B_\mu(\alpha Z)$ can be calculated within the rigorous QED approach [35]. The interaction of the electrons with the Coulomb field of the nucleus is included in the unperturbed Hamiltonian, i.e. the Furry picture is used. The perturbation theory is formulated with the technique of the two-time Green function (TTGF) [41, 42]. To simplify the calculations, the closed $(1s)^2$ shell is regarded as belonging to a redefined vacuum. With this vacuum, the Fourier transform of TTGF can be introduced by

$$\mathcal{G}(E; \vec{x'}; \vec{x})\delta(E - E') = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dx^0 dx'^0 \exp(iE'x'^0 - iEx^0)$$
$$\times \langle 0_{(1s)^2}|T\psi(x'^0, \vec{x'})\psi^\dagger(x^0, \vec{x})|0_{(1s)^2}\rangle, \tag{33}$$

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where $\psi(x^0, \vec{x})$ is the electron-positron field operator in the Heisenberg representation and T is the time-ordered product operator. The energy shift of a state a can be expressed in terms of the TTGF defined by

$$g_{aa}(E) = \langle u_a | \mathcal{G}(E) | u_a \rangle \equiv \int d\vec{x} d\vec{x'} u_a^\dagger(\vec{x'}) \mathcal{G}(E; \vec{x'}; \vec{x}) u_a(\vec{x}), \tag{34}$$

where $u_a(\vec{x})$ is the unperturbed Dirac wave function of the state a. Using the Sz.-Nagy and Kato technique [43], one can derive for the total energy shift $\Delta E_a \equiv E_a - E_a^{(0)}$ [41, 42]

$$\Delta E_a = \frac{\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta E \Delta g_{aa}(E)}{1 + \frac{1}{2\pi i} \oint_\Gamma dE \, \Delta g_{aa}(E)}, \tag{35}$$

where $\Delta E \equiv E - E_a^{(0)}$, $\Delta g_{aa}(E) \equiv g_{aa}(E) - g_{aa}^{(0)}(E)$, and $g_{aa}^{(0)}(E) = (E - E_a^{(0)})^{-1}$. The integrals in the complex E-plane are taken along the contour Γ which surrounds the pole of $g_{aa}(E)$ corresponding to the level a and keeps outside all other singularities. The contour Γ is oriented counter-clockwise.

To first three orders of the perturbation theory, the energy shift is given by

$$\Delta E_a^{(1)} = \frac{1}{2\pi i} \oint_\Gamma dE \, \Delta E \Delta g_{aa}^{(1)}(E), \tag{36}$$

$$\Delta E_a^{(2)} = \frac{1}{2\pi i} \oint_\Gamma dE \, \Delta E \Delta g_{aa}^{(2)}(E) - \left(\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta E \Delta g_{aa}^{(1)}(E) \right) \left(\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta g_{aa}^{(1)}(E) \right), \tag{37}$$

$$\Delta E_a^{(3)} = \frac{1}{2\pi i} \oint_\Gamma dE \, \Delta E \Delta g_{aa}^{(3)}(E) - \left(\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta E \Delta g_{aa}^{(2)}(E) \right) \left(\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta g_{aa}^{(1)}(E) \right)$$
$$- \left(\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta E \Delta g_{aa}^{(1)}(E) \right) \left(\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta g_{aa}^{(2)}(E) \right)$$
$$+ \left(\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta E \Delta g_{aa}^{(1)}(E) \right) \left(\frac{1}{2\pi i} \oint_\Gamma dE \, \Delta g_{aa}^{(1)}(E) \right)^2. \tag{38}$$

The redefinition of the vacuum changes $i0$ to $-i0$ in the electron propagator denominators corresponding to the closed $(1s)^2$ shell. In other words it means replacing the standard Feynman contour of integration over the electron energy C with a new contour C' (Fig. 2). The second-order contribution is defined by the diagrams presented in Fig. 1. Its evaluation according to Eq. (37) yields formula (24). In the formalism under consideration, the lowest-order interelectronic-interaction and the radiative corrections to Eq. (24) are described by the third-order diagrams presented in Fig. 3 and, according to Eq. (38), by some products of the low-order diagrams depicted in Figs. 4 and 5. According to Fig. 2, to separate the interelectronic-interaction corrections, the contour C' must be divided into two parts, C and C_{int}. The integral along the standard Feynman contour C gives the one-electron radiative correction. The integral along the contour C_{int} describes the interaction of the valent electron with the closed shell electrons. Formula (38) allows one to evaluate the interelectronic-interaction correction $B_\mu(\alpha Z)$ [35]. The results of this evaluation will be presented in the next section together with other related corrections to the Breit – Rabi formula.

4 Corrections to the Breit – Rabi formula for the ground state

Now we assume that the Zeeman splitting ΔE_{mag} of the $2s$ HFS levels $F = I - 1/2$ and $F' = I + 1/2$ is much smaller than the distance to other levels but is comparable with $\Delta E_{\text{HFS}}^{(2s)}$. The unperturbed eigenstates form a two-dimensional subspace $\Omega = \{|1^{(0)}\rangle, |2^{(0)}\rangle\}$, where $|1^{(0)}\rangle = |20\frac{1}{2}IFM_F\rangle$, $|2^{(0)}\rangle = |20\frac{1}{2}IF'M_F\rangle$. Employing the perturbation theory for degenerate states [42] with energy ε_v we denote the projector on Ω by

$$P^{(0)} = \sum_{i=1}^{2} |i^{(0)}\rangle\langle i^{(0)}| \,. \tag{39}$$

We project the Green function $\mathcal{G}(E)$ on the subspace Ω

$$g(E) = P^{(0)}\mathcal{G}(E)P^{(0)} \,, \tag{40}$$

where, as in Eq. (34), the integration over the electron coordinates is implicit. In this case we can choose a contour Γ in the complex E-plane in a way that it surrounds all $g(E)$ poles, which correspond to the states under consideration, and keeps outside all other singularities of $g(E)$. As in the case of a single level, to the zeroth-order approximation one easily finds

$$g^{(0)}(E) = \sum_{i=1}^{2} \frac{|i^{(0)}\rangle\langle i^{(0)}|}{E - E_i^{(0)}} \,. \tag{41}$$

We introduce the operators K and P by

$$K \equiv \frac{1}{2\pi i} \oint_{\Gamma} dE \, E g(E) \,, \tag{42}$$

$$P \equiv \frac{1}{2\pi i} \oint_{\Gamma} dE \, g(E) \,. \tag{43}$$

As it is shown in Ref. [42], the energy levels are determined from the equation

$$\det(H - E) = 0 \,, \tag{44}$$

where

$$H = P^{-\frac{1}{2}}KP^{-\frac{1}{2}} \,. \tag{45}$$

The operators K and P are constructed by formulas (42) and (43)

$$K = K^{(0)} + K^{(1)} + K^{(2)} + K^{(3)} + \dots \,, \tag{46}$$

$$P = P^{(0)} + P^{(1)} + P^{(2)} + P^{(3)} + \dots \,, \tag{47}$$

where the superscript indicates the order of the perturbation theory in a small parameter. The operator H is

$$H = H^{(0)} + H^{(1)} + H^{(2)} + H^{(3)} + \dots \,, \tag{48}$$

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where

$$H^{(0)} = K^{(0)} \,, \tag{49}$$

$$H^{(1)} = K^{(1)} - \frac{1}{2}P^{(1)}K^{(0)} - \frac{1}{2}K^{(0)}P^{(1)} \,, \tag{50}$$

$$
\begin{aligned}
H^{(2)} = {} & K^{(2)} - \frac{1}{2}P^{(2)}K^{(0)} - \frac{1}{2}K^{(0)}P^{(2)} - \frac{1}{2}P^{(1)}K^{(1)} - \frac{1}{2}K^{(1)}P^{(1)} \\
& + \frac{3}{8}P^{(1)}P^{(1)}K^{(0)} + \frac{3}{8}K^{(0)}P^{(1)}P^{(1)} + \frac{1}{4}P^{(1)}K^{(0)}P^{(1)} \,,
\end{aligned}
\tag{51}
$$

$$
\begin{aligned}
H^{(3)} = {} & K^{(3)} - \frac{1}{2}P^{(3)}K^{(0)} - \frac{1}{2}K^{(0)}P^{(3)} - \frac{1}{2}P^{(1)}K^{(2)} - \frac{1}{2}K^{(2)}P^{(1)} - \frac{1}{2}P^{(2)}K^{(1)} - \frac{1}{2}K^{(1)}P^{(2)} \\
& + \frac{3}{8}P^{(1)}P^{(2)}K^{(0)} + \frac{3}{8}K^{(0)}P^{(1)}P^{(2)} + \frac{3}{8}P^{(2)}P^{(1)}K^{(0)} + \frac{3}{8}K^{(0)}P^{(2)}P^{(1)} \\
& + \frac{1}{4}P^{(1)}K^{(0)}P^{(2)} + \frac{1}{4}P^{(2)}K^{(0)}P^{(1)} + \frac{3}{8}P^{(1)}P^{(1)}K^{(1)} + \frac{3}{8}K^{(1)}P^{(1)}P^{(1)} + \frac{1}{4}P^{(1)}K^{(1)}P^{(1)} \\
& - \frac{5}{16}P^{(1)}P^{(1)}P^{(1)}K^{(0)} - \frac{5}{16}K^{(0)}P^{(1)}P^{(1)}P^{(1)} \\
& - \frac{3}{16}P^{(1)}P^{(1)}K^{(0)}P^{(1)} - \frac{3}{16}P^{(1)}K^{(0)}P^{(1)}P^{(1)} \,.
\end{aligned}
\tag{52}
$$

Taking into account only the relevant contributions of kind $\alpha \times \mu/\mu_N \times B$ and $\alpha \times B \times B$, where α comes from the interelectronic interaction, we obtain for the third-order term in Eq. (48)

$$
\begin{aligned}
H^{(3)}_{jk} = {} & \frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta E\Delta g^{(3)}_{jk}(E) - \frac{1}{2}\sum_{l=1}^{2}\left[\left(\frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta g^{(1)}_{jl}(E)\right)\left(\frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta E\Delta g^{(2)}_{lk}(E)\right)\right. \\
& \left. + \left(\frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta E\Delta g^{(2)}_{jl}(E)\right)\left(\frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta g^{(1)}_{lk}(E)\right)\right] \\
& - \frac{1}{2}\sum_{l=1}^{2}\left[\left(\frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta g^{(2)}_{jl}(E)\right)\left(\frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta E\Delta g^{(1)}_{lk}(E)\right)\right. \\
& \left. + \left(\frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta E\Delta g^{(1)}_{jl}(E)\right)\left(\frac{1}{2\pi i}\oint_{\Gamma} dE\,\Delta g^{(2)}_{lk}(E)\right)\right] \,,
\end{aligned}
\tag{53}
$$

where $\Delta E \equiv E - \varepsilon_v$, $j, k = 1, 2$.

Keeping only the three lowest-order terms in B, we get the following equation for the perturbed energies:

$$
\begin{vmatrix}
h_0(F) + h_1(F)B + h_2(F)B^2 - E & \tilde{h}_1(F, F')B + \tilde{h}_2(F, F')B^2 \\
\tilde{h}_1(F', F)B + \tilde{h}_2(F', F)B^2 & h_0(F') + h_1(F')B + h_2(F')B^2 - E
\end{vmatrix} = 0 \,.
\tag{54}
$$

Here $F = I - \frac{1}{2}$, $F' = I + \frac{1}{2}$,

$$h_0(k) = E(k) \tag{55}$$

is the energy of the HFS level,

$$
\begin{aligned}
h_1(k) = {} & \frac{1}{B}[\Delta E^{(1)}_{(\vec{B})}(k, k) + \Delta E^{(2)}_{(\mu)}(k, k) + \Delta E^{(2)}_{(Q)}(k, k) + \Delta E^{(3)}_{(\mu)}(k, k) + \Delta E^{(3)}_{(Q)}(k, k)] \\
& + (\Delta g_{\mathrm{int}} + \Delta g_{\mathrm{QED}} + \Delta g^{(e)}_{\mathrm{rec}} + \Delta g_{\mathrm{NS}} + \Delta g_{\mathrm{NP}})Y_{\mathrm{el}}(k)\mu_0 M_F - \Delta g^{(n)}_{\mathrm{rec}}Y^{(\mu)}_{\mathrm{nuc}}(k)\mu_N M_F \\
& = g(k)\mu_0 M_F \,,
\end{aligned}
\tag{56}
$$

$$h_2(k) = \frac{1}{B^2}[\Delta E^{(2)}_{(\vec{B})}(k,k) + \Delta E^{(3)}_{(\vec{B})}(k,k)]\,, \tag{57}$$

$$\tilde{h}_1(j,k) = \frac{1}{B}[\Delta E^{(1)}_{(\vec{B})}(j,k) + \Delta E^{(2)}_{(\mu)}(j,k) + \Delta E^{(2)}_{(Q)}(j,k) + \Delta E^{(3)}_{(\mu)}(j,k) + \Delta E^{(3)}_{(Q)}(j,k)]$$
$$+ (\Delta_{\text{int}} + \Delta_{\text{QED}} + \Delta^{(e)}_{\text{rec}} + \Delta_{\text{NS}} + \Delta_{\text{NP}})\mu_0 - \Delta^{(n)}_{\text{rec}}\mu_N\,, \tag{58}$$

$$\tilde{h}_2(j,k) = \frac{1}{B^2}[\Delta E^{(2)}_{(\vec{B})}(j,k) + \Delta E^{(3)}_{(\vec{B})}(j,k)]\,, \tag{59}$$

where $j, k = F, F'$. Δ_{int}, Δ_{QED}, $\Delta^{(e)}_{\text{rec}}$, Δ_{NS}, and Δ_{NP} are the interelectronic-interaction, QED, nuclear recoil, nuclear size, and nuclear polarization corrections. They are similar to the corresponding corrections to $h_1(k)$ but have a different angular factor as well as $\Delta^{(n)}_{\text{rec}}$. It should be noted that we have neglected here terms describing virtual transitions into excited nuclear states via the direct interaction of the nucleus with the magnetic field [22]. The energy shifts are

$$\Delta E^{(1)}_{(\vec{B})}(j,k) = \sum_{m_j M_I} \sum_{m'_j M'_I} C^{jM_F}_{\frac{1}{2}m_j I M_I} C^{kM_F}_{\frac{1}{2}m'_j I M'_I} \langle IM_I|V_{\vec{B}}|IM'_I\rangle\,, \tag{60}$$

$$\Delta E^{(2)}_{(\mu,Q,\vec{B})}(j,k) = \sum_{m_j M_I} \sum_{m'_j M'_I} C^{jM_F}_{\frac{1}{2}m_j I M_I} C^{kM_F}_{\frac{1}{2}m'_j I M'_I} \langle IM_I|I^{(2)}_{\mu,Q,\vec{B}}|IM'_I\rangle\,, \tag{61}$$

$$\Delta E^{(3)}_{(\mu,Q,\vec{B})}(j,k) = \sum_{m_j M_I} \sum_{m'_j M'_I} C^{jM_F}_{\frac{1}{2}m_j I M_I} C^{kM_F}_{\frac{1}{2}m'_j I M'_I} \langle IM_I|I^{(3a)}_{\mu,Q,\vec{B}} + I^{(3b)}_{\mu,Q,\vec{B}} + I^{(3c)}_{\mu,Q,\vec{B}} + I^{(3d)}_{\mu,Q,\vec{B}}|IM'_I\rangle\,, \tag{62}$$

where

$$I^{(2)}_{\mu,Q,\vec{B}} = 2f \sum_n^{(\epsilon_n \neq \epsilon_v)} \frac{\langle v|V^{(e)}_{\vec{B}}|n\rangle\langle n|W|v'\rangle}{\varepsilon_v - \varepsilon_n}\,, \tag{63}$$

$$I_{\mu,Q,\vec{B}}^{(3a)} = f \sum_{\varepsilon_c=E_{1,-1}} \left(\sum_{n_1,n_2}^{(\varepsilon_{n_1}\neq\varepsilon_v, \varepsilon_{n_2}\neq\varepsilon_v)} \frac{2}{(\varepsilon_v-\varepsilon_{n_1})(\varepsilon_v-\varepsilon_{n_2})} \left[\langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1|W|n_2\rangle\langle n_2 c|I(0)|v'c\rangle \right.\right.$$

$$\left. + \langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1 c|I(0)|n_2 c\rangle\langle n_2|W|v'\rangle + \langle v|W|n_1\rangle\langle n_1|V_{\vec{B}}^{(e)}|n_2\rangle\langle n_2 c|I(0)|v'c\rangle \right]$$

$$- \sum_{\varepsilon_{\tilde{v}}=\varepsilon_v} \sum_n^{(\varepsilon_n\neq\varepsilon_v)} \frac{2}{(\varepsilon_v-\varepsilon_n)^2} \left[\langle v|V_{\vec{B}}^{(e)}|n\rangle\langle n|W|\tilde{v}\rangle\langle\tilde{v}c|I(0)|v'c\rangle \right.$$

$$\left.\left. + \langle v|V_{\vec{B}}^{(e)}|n\rangle\langle nc|I(0)|\tilde{v}c\rangle\langle\tilde{v}|W|v'\rangle + \langle v|V_{\vec{B}}^{(e)}|\tilde{v}\rangle\langle\tilde{v}|W|n\rangle\langle nc|I(0)|v'c\rangle \right] \right), \tag{64}$$

$$I_{\mu,Q,\vec{B}}^{(3b)} = -f \sum_{\varepsilon_c=E_{1,-1}} \left(\sum_{n_1,n_2}^{(\varepsilon_{n_1}\neq\varepsilon_v, \varepsilon_{n_2}\neq\varepsilon_v)} \frac{2}{(\varepsilon_v-\varepsilon_{n_1})(\varepsilon_v-\varepsilon_{n_2})} \left[\langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1|W|n_2\rangle\langle n_2 c|I(\omega)|cv'\rangle \right.\right.$$

$$\left. + \langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1 c|I(\omega)|cn_2\rangle\langle n_2|W|v'\rangle + \langle v|W|n_1\rangle\langle n_1|V_{\vec{B}}^{(e)}|n_2\rangle\langle n_2 c|I(\omega)|cv'\rangle \right]$$

$$- \sum_{\varepsilon_{\tilde{v}}=\varepsilon_v} \sum_n^{(\varepsilon_n\neq\varepsilon_v)} \frac{2}{(\varepsilon_v-\varepsilon_n)^2} \left[\langle v|V_{\vec{B}}^{(e)}|n\rangle\langle n|W|\tilde{v}\rangle\langle\tilde{v}c|I(\omega)|cv'\rangle \right.$$

$$\left. + \langle v|V_{\vec{B}}^{(e)}|n\rangle\langle nc|I(\omega)|c\tilde{v}\rangle\langle\tilde{v}|W|v'\rangle + \langle v|V_{\vec{B}}^{(e)}|\tilde{v}\rangle\langle\tilde{v}|W|n\rangle\langle nc|I(\omega)|cv'\rangle \right]$$

$$+ \sum_{\varepsilon_{\tilde{v}}=\varepsilon_v} \sum_n^{(\varepsilon_n\neq\varepsilon_v)} \frac{2}{\varepsilon_v-\varepsilon_n} \left[\langle v|V_{\vec{B}}^{(e)}|n\rangle\langle n|W|\tilde{v}\rangle\langle\tilde{v}c|I'(\omega)|cv'\rangle \right.$$

$$\left. + \langle v|V_{\vec{B}}^{(e)}|n\rangle\langle nc|I'(\omega)|c\tilde{v}\rangle\langle\tilde{v}|W|v'\rangle + \langle v|V_{\vec{B}}^{(e)}|\tilde{v}\rangle\langle\tilde{v}|W|n\rangle\langle nc|I'(\omega)|cv'\rangle \right]$$

$$\left. + \sum_{\varepsilon_{\tilde{v}}=\varepsilon_v} \sum_{\varepsilon_{\check{v}}=\varepsilon_v} \langle v|V_{\vec{B}}^{(e)}|\tilde{v}\rangle\langle\tilde{v}c|I''(\omega)|c\check{v}\rangle\langle\check{v}|W|v'\rangle \right), \tag{65}$$

$$I_{\mu,Q,\vec{B}}^{(3c)} = f \sum_{\varepsilon_c=E_{1,-1}} \left(\sum_{n_1,n_2}^{(\varepsilon_{n_1}\neq\varepsilon_v, \varepsilon_{n_2}\neq\varepsilon_c)} \frac{2}{(\varepsilon_v-\varepsilon_{n_1})(\varepsilon_c-\varepsilon_{n_2})} \left[\langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle c|W|n_2\rangle\langle n_1 n_2|I(0)|v'c\rangle \right.\right.$$

$$+ \langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1 c|I(0)|v'n_2\rangle\langle n_2|W|c\rangle + \langle v|W|n_1\rangle\langle c|V_{\vec{B}}^{(e)}|n_2\rangle\langle n_1 n_2|I(0)|v'c\rangle$$

$$\left. + \langle v|W|n_1\rangle\langle n_1 c|I(0)|v'n_2\rangle\langle n_2|V_{\vec{B}}^{(e)}|c\rangle \right]$$

$$+ \sum_{n_1,n_2}^{(\varepsilon_{n_1}\neq\varepsilon_c, \varepsilon_{n_2}\neq\varepsilon_c)} \frac{2}{(\varepsilon_c-\varepsilon_{n_1})(\varepsilon_c-\varepsilon_{n_2})} \left[\langle c|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1|W|n_2\rangle\langle n_2 v|I(0)|cv'\rangle \right.$$

$$\left. + \langle c|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1 v|I(0)|n_2 v'\rangle\langle n_2|W|c\rangle + \langle c|W|n_1\rangle\langle n_1|V_{\vec{B}}^{(e)}|n_2\rangle\langle n_2 v|I(0)|cv'\rangle \right]$$

$$- \sum_{\varepsilon_{\tilde{c}}=E_{1,-1}} \sum_n^{(\varepsilon_n\neq\varepsilon_c)} \frac{2}{(\varepsilon_c-\varepsilon_n)^2} \left[\langle c|V_{\vec{B}}^{(e)}|n\rangle\langle n|W|\tilde{c}\rangle\langle\tilde{c}v|I(0)|cv'\rangle \right.$$

$$\left.\left. + \langle c|V_{\vec{B}}^{(e)}|n\rangle\langle nv|I(0)|\tilde{c}v'\rangle\langle\tilde{c}|W|c\rangle + \langle c|V_{\vec{B}}^{(e)}|\tilde{c}\rangle\langle\tilde{c}|W|n\rangle\langle nv|I(0)|cv'\rangle \right] \right), \tag{66}$$

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$$I_{\mu,Q,\vec{B}}^{(3d)} = -f \sum_{\varepsilon_c=E_{1,-1}} \left(\sum_{n_1,n_2}^{(\varepsilon_{n_1}\neq\varepsilon_v,\,\varepsilon_{n_2}\neq\varepsilon_c)} \frac{2}{(\varepsilon_v-\varepsilon_{n_1})(\varepsilon_c-\varepsilon_{n_2})} \left[\langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle c|W|n_2\rangle\langle n_1 n_2|I(\omega)|cv'\rangle \right.\right.$$

$$+ \langle v|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1 c|I(\omega)|n_2 v'\rangle\langle n_2|W|c\rangle + \langle v|W|n_1\rangle\langle c|V_{\vec{B}}^{(e)}|n_2\rangle\langle n_1 n_2|I(\omega)|cv'\rangle$$

$$+ \langle v|W|n_1\rangle\langle n_1 c|I(\omega)|n_2 v'\rangle\langle n_2|V_{\vec{B}}^{(e)}|c\rangle \Big]$$

$$+ \sum_{n_1,n_2}^{(\varepsilon_{n_1}\neq\varepsilon_c,\,\varepsilon_{n_2}\neq\varepsilon_c)} \frac{2}{(\varepsilon_c-\varepsilon_{n_1})(\varepsilon_c-\varepsilon_{n_2})} \left[\langle c|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1|W|n_2\rangle\langle n_2 v|I(\omega)|v'c\rangle \right.$$

$$+ \langle c|V_{\vec{B}}^{(e)}|n_1\rangle\langle n_1 v|I(\omega)|v'n_2\rangle\langle n_2|W|c\rangle + \langle c|W|n_1\rangle\langle n_1|V_{\vec{B}}^{(e)}|n_2\rangle\langle n_2 v|I(\omega)|v'c\rangle \Big]$$

$$- \sum_{\varepsilon_{\tilde{c}}=E_{1,-1}} \sum_n^{(\varepsilon_n\neq\varepsilon_c)} \frac{2}{(\varepsilon_c-\varepsilon_n)^2} \left[\langle c|V_{\vec{B}}^{(e)}|n\rangle\langle n|W|\tilde{c}\rangle\langle \tilde{c}v|I(\omega)|v'c\rangle \right.$$

$$+ \langle c|V_{\vec{B}}^{(e)}|n\rangle\langle nv|I(\omega)|v'\tilde{c}\rangle\langle \tilde{c}|W|c\rangle + \langle c|V_{\vec{B}}^{(e)}|\tilde{c}\rangle\langle \tilde{c}|W|n\rangle\langle nv|I(\omega)|v'c\rangle \Big]$$

$$- \sum_{\varepsilon_{\tilde{c}}=E_{1,-1}} \sum_n^{(\varepsilon_n\neq\varepsilon_c)} \frac{2}{\varepsilon_c-\varepsilon_n} \left[\langle c|V_{\vec{B}}^{(e)}|n\rangle\langle n|W|\tilde{c}\rangle\langle \tilde{c}v|I'(\omega)|v'c\rangle \right.$$

$$+ \langle c|V_{\vec{B}}^{(e)}|n\rangle\langle nv|I'(\omega)|v'\tilde{c}\rangle\langle \tilde{c}|W|c\rangle + \langle c|V_{\vec{B}}^{(e)}|\tilde{c}\rangle\langle \tilde{c}|W|n\rangle\langle nv|I'(\omega)|v'c\rangle \Big]$$

$$- \sum_{\varepsilon_{\tilde{c}}=E_{1,-1}} \sum_n^{(\varepsilon_n\neq\varepsilon_v)} \frac{2}{\varepsilon_v-\varepsilon_n} \left[\langle v|V_{\vec{B}}^{(e)}|n\rangle\langle nc|I'(\omega)|\tilde{c}v'\rangle\langle \tilde{c}|W|c\rangle + \langle v|W|n\rangle\langle nc|I'(\omega)|\tilde{c}v'\rangle\langle \tilde{c}|V_{\vec{B}}^{(e)}|c\rangle \right]$$

$$+ \sum_{\varepsilon_{\tilde{v}}=\varepsilon_v} \sum_n^{(\varepsilon_n\neq\varepsilon_c)} \frac{2}{\varepsilon_c-\varepsilon_n} \left[\langle v|V_{\vec{B}}^{(e)}|\tilde{v}\rangle\langle \tilde{v}c|I'(\omega)|nv'\rangle\langle n|W|c\rangle + \langle v|W|\tilde{v}\rangle\langle \tilde{v}c|I'(\omega)|nv'\rangle\langle n|V_{\vec{B}}^{(e)}|c\rangle \right]$$

$$- \sum_{\varepsilon_{\tilde{v}}=\varepsilon_v} \sum_{\varepsilon_{\tilde{c}}=E_{1,-1}} \left[\langle v|V_{\vec{B}}^{(e)}|\tilde{v}\rangle\langle \tilde{v}c|I''(\omega)|\tilde{c}v'\rangle\langle \tilde{c}|W|c\rangle + \langle v|W|\tilde{v}\rangle\langle \tilde{v}c|I''(\omega)|\tilde{c}v'\rangle\langle \tilde{c}|V_{\vec{B}}^{(e)}|c\rangle \right]$$

$$+ \sum_{\varepsilon_{\tilde{c}}=E_{1,-1}} \sum_{\varepsilon_{\check{c}}=E_{1,-1}} \langle c|V_{\vec{B}}^{(e)}|\tilde{c}\rangle\langle \tilde{c}v|I''(\omega)|v'\check{c}\rangle\langle \check{c}|W|c\rangle \Bigg) . \tag{67}$$

Here

$$f = \begin{cases} 1 & \text{for } W = V_{\text{HFS}}^{(\mu)} \text{ or } W = V_{\text{HFS}}^{(Q)} \\ \frac{1}{2} & \text{for } W = V_{\vec{B}}^{(e)} \end{cases}, \tag{68}$$

$$\langle n_1 n_2|I(\omega)|n_3 n_4\rangle \equiv \int d\vec{x}_1 d\vec{x}_2\, u_{n_1}^\dagger(\vec{x}_1) u_{n_2}^\dagger(\vec{x}_2) I(\omega) u_{n_3}(\vec{x}_1) u_{n_4}(\vec{x}_2) , \tag{69}$$

$$I(\omega) = \alpha \frac{(1-\vec{\alpha}_1\cdot\vec{\alpha}_2)\cos(\omega r_{12})}{r_{12}} , \tag{70}$$

$$I'(\omega) = \frac{dI(\omega)}{d\omega} , \quad I''(\omega) = \frac{d^2 I(\omega)}{d\omega^2} , \tag{71}$$

$\omega = \varepsilon_v - E_{1,-1}$, and $r_{12} = |\vec{x}_1 - \vec{x}_2|$. As in the case of evaluation of $\delta g_{\text{HFS}}^{(2s)}$ considered above, the diagrams corresponding to Eq. (61) are presented in Fig. 1 and the ones corresponding to Eq. (62) are presented in Figs. 3 – 5. Separating the interelectronic-interaction corrections is carried out according to Fig. 2 just as it was done in section 3.

The calculation of $h_1(k)$ was discussed in detail in Ref. [35]. We found that

$$h_1(k)B = M_F \left[g_j Y_{\text{el}}(k) - g_I' Y_{\text{nuc}}^{(\mu)}(k) \right.$$
$$\left. + \alpha^2 Z \frac{1}{12} \left\{ g_I' Y_{\text{nuc}}^{(\mu)}(k) S_2^{(t)}(\alpha Z) + (\alpha Z)^2 \frac{23}{180} Q \left(\frac{m_e c}{\hbar} \right)^2 Y_{\text{nuc}}^{(Q)}(k) T_2^{(t)}(\alpha Z) \right\} \right] \mu_0 B. \quad (72)$$

Calculating the other matrix elements, we obtain

$$h_2(k)B^2 = \frac{14}{(\alpha Z)^2} U_2^{(t)}(\alpha Z)(\mu_0 B)^2/(m_e c^2), \quad (73)$$

$$\tilde{h}_1(j,k)B = \frac{1}{2} \frac{\sqrt{(I+1/2)^2 - M_F^2}}{I+1/2} \left[g_j + g_I' \right.$$
$$\left. - \alpha^2 Z \frac{1}{12} \left\{ g_I' S_2^{(t)}(\alpha Z) + (\alpha Z)^2 \frac{23}{360} Q \left(\frac{m_e c}{\hbar} \right)^2 \frac{2I+3}{2I} T_2^{(t)}(\alpha Z) \right\} \right] \mu_0 B, \quad (74)$$

$$\tilde{h}_2(j,k) = 0. \quad (75)$$

Here the total functions are

$$U_2^{(t)}(\alpha Z) = U_2(\alpha Z) + \frac{1}{Z} B_{\vec{B}}(\alpha Z) + \frac{1}{Z^2} C_{\vec{B}}(\alpha Z) + \ldots, \quad (76)$$

$$S_2^{(t)}(\alpha Z) = S_2(\alpha Z) + \frac{1}{Z} B_\mu(\alpha Z) + \frac{1}{Z^2} C_\mu(\alpha Z) + \ldots, \quad (77)$$

$$T_2^{(t)}(\alpha Z) = T_2(\alpha Z) + \frac{1}{Z} B_Q(\alpha Z) + \frac{1}{Z^2} C_Q(\alpha Z) + \ldots. \quad (78)$$

It must be stressed that the contributions of order $1/Z^2$ and higher to these functions are not included in Eq. (54). Their evaluation would require consideration of some higher-order terms in operator (48). The expansions (76) – (78) are presented by anology with Eqs. (26) and (27). The function

$$U_2(\alpha Z) = \frac{(\alpha Z)^2 m_e c^2}{14(\mu_0 B)^2} \Delta E_{(\vec{B})}^{(2)}(F, F) \quad (79)$$

determines the one-electron contribution. Calculations employing Eqs. (64) – (67) yield for the interelectronic-interaction corrections $B_{\vec{B}}(\alpha Z)$, $B_\mu(\alpha Z)$, and $B_Q(\alpha Z)$

$$B_{\vec{B}}(\alpha Z) = \frac{\alpha^2 Z^3 m_e c^2}{14(\mu_0 B)^2} \Delta E_{(\vec{B})}^{(3)}(F, F), \quad (80)$$

$$B_\mu(\alpha Z) = \frac{12}{\alpha^2 \frac{m_e}{m_p} g_I Y_{\text{nuc}}^{(\mu)}(F)} \frac{\Delta E_{(\mu)}^{(3)}(F, F)}{\mu_0 B M_F}, \quad (81)$$

$$B_Q(\alpha Z) = \frac{2160}{23 \alpha^4 Z^2 Q \left(\frac{m_e c}{\hbar} \right)^2 Y_{\text{nuc}}^{(Q)}(F)} \frac{\Delta E_{(Q)}^{(3)}(F, F)}{\mu_0 B M_F}. \quad (82)$$

It must be noted that, because of the smallness of the contribution determined by $B_Q(\alpha Z)$, only $B_{\vec{B}}(\alpha Z)$ and $B_\mu(\alpha Z)$ were evaluated in the present paper. For checking purposes the calculation of these functions was performed in both Feynman and Coulomb gauges. The results of both calculations coincide with each other.

Solving equation (54), we finally obtain for $M_F = -I + 1/2, ..., I - 1/2$,

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left[a_1(1 + \epsilon_1)M_F x + \epsilon_2 \frac{\Delta E_{\text{HFS}}^{(2s)}}{m_e c^2} x^2 \right.$$
$$\left. \pm \frac{1}{2} \sqrt{1 + \frac{4M_F}{2I + 1} c_1(1 + \delta_1)x + c_2(1 + \delta_2 + M_F^2 \delta_3)x^2} \right]. \quad (83)$$

Here

$$\epsilon_1 = -\frac{1}{2g_I'} [\delta g_{\text{HFS}}^{(2s)}(F) + \delta g_{\text{HFS}}^{(2s)}(F + 1)]$$
$$= -\alpha^2 Z \frac{1}{12} \left[S_2^{(t)}(\alpha Z) - (\alpha Z)^2 \frac{23Q}{120 g_I'} \left(\frac{m_e c}{\hbar} \right)^2 \frac{1}{I(2I - 1)} T_2^{(t)}(\alpha Z) \right], \quad (84)$$

$$\epsilon_2 = \frac{14}{(\alpha Z)^2} U_2^{(t)}(\alpha Z), \quad (85)$$

$$\delta_1 = \frac{2I + 1}{2(g_j + g_I')} [\delta g_{\text{HFS}}^{(2s)}(F + 1) - \delta g_{\text{HFS}}^{(2s)}(F)]$$
$$= -\alpha^2 Z \frac{1}{12(g_j + g_I')} \left[g_I' S_2^{(t)}(\alpha Z) - (\alpha Z)^2 \frac{23}{360} Q \left(\frac{m_e c}{\hbar} \right)^2 \frac{4I^2 + 4I + 3}{I(2I - 1)} T_2^{(t)}(\alpha Z) \right], \quad (86)$$

$$\delta_2 = -\alpha^2 Z \frac{1}{6(g_j + g_I')} \left[g_I' S_2^{(t)}(\alpha Z) + (\alpha Z)^2 \frac{23}{360} Q \left(\frac{m_e c}{\hbar} \right)^2 \frac{2I + 3}{2I} T_2^{(t)}(\alpha Z) \right], \quad (87)$$

$$\delta_3 = \frac{1}{g_j + g_I'} \alpha^4 Z^3 \frac{23}{360} Q \left(\frac{m_e c}{\hbar} \right)^2 \frac{1}{I(2I - 1)} T_2^{(t)}(\alpha Z). \quad (88)$$

For $F' = I + \frac{1}{2}$ and $M_F = \pm(I + \frac{1}{2})$, in contrast to Eq. (9), we have

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left[\frac{1}{2} \pm d_1(1 + \eta_1)x + \eta_2 \frac{\Delta E_{\text{HFS}}^{(2s)}}{m_e c^2} x^2 \right], \quad (89)$$

where

$$\eta_1 = \alpha^2 Z \frac{1}{6(g_j - 2I g_I')} \left[g_I' I S_2^{(t)}(\alpha Z) + (\alpha Z)^2 \frac{23}{360} Q \left(\frac{m_e c}{\hbar} \right)^2 T_2^{(t)}(\alpha Z) \right], \quad (90)$$

$$\eta_2 = \epsilon_2 = \frac{14}{(\alpha Z)^2} U_2^{(t)}(\alpha Z), \quad (91)$$

and the "$-$" and "$+$" signs correspond to $M_F = -(I + \frac{1}{2})$ and $M_F = I + \frac{1}{2}$, respectively.

If $I = 1/2$, the electrical quadrupole interaction vanishes and one can easily obtain for $M_F = 0$:

$$\Delta E_{\text{mag}}(x) = \Delta E_{\text{HFS}}^{(2s)} \left[\epsilon_2 \frac{\Delta E_{\text{HFS}}^{(2s)}}{m_e c^2} x^2 \pm \frac{1}{2} \sqrt{1 + c_2(1 + \delta_2)x^2} \right] \quad (92)$$

with

$$\delta_2 = -\frac{g_I'}{6(g_j + g_I')} \alpha^2 Z S_2^{(t)}(\alpha Z). \quad (93)$$

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For $I = 1/2$, $M_F = \pm 1$, the effect is described by formula (89) with

$$\eta_1 = \frac{g_I'}{12(g_j - g_I')} \alpha^2 Z S_2^{(\mathrm{t})}(\alpha Z) \,. \tag{94}$$

5 Numerical results

In Table 1, we present the numerical results for the functions $U_2(\alpha Z)$, $B_{\vec{B}}(\alpha Z)$, $U_2^{(\mathrm{t})}(\alpha Z)$, $S_2(\alpha Z)$, $B_\mu(\alpha Z)$, $S_2^{(\mathrm{t})}(\alpha Z)$, and $T_2(\alpha Z)$ (only for the isotopes with $I > 1/2$) defined by Eqs. (79), (80), (76), (29), (81), (77), and (30), respectively, for the $2s$ state. All the values are calculated for the extended nuclear charge distribution. The root-mean-square nuclear charge radii $\langle r^2 \rangle^{1/2}$ were taken from Ref. [44]. For those elements for which no accurate experimental radii were available we employed the empirical expression [45]

$$\langle r^2 \rangle^{1/2} = 0.836 A^{1/3} + 0.570 (\pm 0.05) \ \mathrm{fm} \,, \tag{95}$$

where A is the nuclear mass expressed in a.m.u. The calculations were performed using the dual-kinetic-balance (DKB) basis set method [46] with the basis functions constructed from B-splines [47, 48]. The uncertainties of $U_2(\alpha Z)$, $B_{\vec{B}}(\alpha Z)$, $S_2(\alpha Z)$, $B_\mu(\alpha Z)$, and $T_2(\alpha Z)$ were estimated by adding quadratically two errors, one obtained by varying $\langle r^2 \rangle^{1/2}$ within its uncertainty and the other obtained by changing the model of the nuclear-charge distribution from the Fermi to the homogeneously-charged-sphere model. The uncertainties of the total functions $U_2^{(\mathrm{t})}(\alpha Z)$ and $S_2^{(\mathrm{t})}(\alpha Z)$ due to uncalculated second- and higher-order terms were estimated as the first-order correction ($\sim B_{\vec{B}}(\alpha Z)/Z$ and $\sim B_\mu(\alpha Z)/Z$, respectively) multiplied by the factor $2/Z$. The uncertainty due to uncalculated first- and higher-order terms in Eq. (78) was estimated in a similar way.

In Table 2, we present the individual contributions to the $2s$ g_j factor for some Li-like ions with $I \neq 0$ in the range $Z = 6 - 32$. The Dirac point-nucleus value is obtained by Eq. (7). The interelectronic-interaction (Δg_{int}), QED (Δg_{QED}), nuclear-recoil ($\Delta g_{\mathrm{rec}}^{(e)}$), and nuclear-size ($\Delta g_{\mathrm{NS}}$) corrections are obtained as described in Refs. [32, 33]. The nuclear-size correction was evaluated for the homogeneously-charged-sphere model if $Z = 6 - 16$ and for the Fermi model if $Z = 20 - 32$. The nuclear polarization contribution to the $2s$ g_j factor of light Li-like ions can be neglected [17]. The g_j factor values given in Table 2 are used for calculations of the coefficients in the Breit – Rabi formula.

In Table 3, the numerical results for the coefficients in Eqs. (2), (9), (11), (83), (89), and (92) are listed for some Li-like isotopes in the interval $Z = 6 - 32$. Since in all the cases under consideration the absolute value of the recoil correction to the bound-nucleus g_I factor is smaller than 10^{-11} [12], we actually have in Eq. (8): $g_I' = \frac{m_e}{m_p} g_I$.

6 Discussion

The energy separation between the ground-state HFS components ($F = I - 1/2$ and $F' = I + 1/2$) of a lithiumlike ion can be written as [49]

$$\Delta E_{\text{HFS}}^{(2s)} = \frac{1}{6}\alpha(\alpha Z)^3 \frac{\mu}{\mu_N} \frac{m_e}{m_p} \frac{2I+1}{2I} m_e c^2$$
$$\times \left\{ [A^{(2s)}(\alpha Z)(1 - \delta^{(2s)}(1 - \epsilon^{(2s)}) + x_{\text{rad}}^{(2s)}] \right.$$
$$\left. + \frac{1}{Z}B^{(2s)}(\alpha Z) + \frac{1}{Z^2}C^{(2s)}(\alpha Z) + \dots \right\}, \tag{96}$$

where

$$A^{(2s)}(\alpha Z) = \frac{2[2(1+\gamma) + \sqrt{2(1+\gamma)}]}{(1+\gamma)^2\gamma(4\gamma^2-1)} = 1 + \frac{17}{8}(\alpha Z)^2 + \frac{449}{128}(\alpha Z)^4 + \dots \tag{97}$$

is the one-electron relativistic factor, $\delta^{(2s)}$ is the nuclear charge distribution correction, $\epsilon^{(2s)}$ is the nuclear magnetization distribution correction (the Bohr – Weisskopf effect), $x_{\text{rad}}^{(2s)}$ is the QED correction, $B^{(2s)}(\alpha Z)$ and $C^{(2s)}(\alpha Z)$ determine the interelectronic-interaction corrections to the hyperfine structure. Therefore, the dimensionless variable $x = \mu_0 B/\Delta E_{\text{HFS}}^{(2s)}$ is of order of $6\mu_0 B/[\alpha(\alpha Z)^3\frac{m_e}{m_p}m_e c^2]$. The intervals of B and Z, for which $x \sim 1$, are of special interest (in the original paper [36] the fields with $0.1 \leqslant x \leqslant 3$ were considered to be intermediate).

For the magnetic fields with the magnitude $B \sim 1 - 10\,T$, that are generally used in this kind of experiments, Li-like ions with $Z = 6 - 32$ meet the requirement $x \sim 1$. For this reason, only such ions are presented in Tables 1 – 3.

For ions with $Z \leq 32$, the electric-quadrupole corrections to the coefficients a_1, c_1, c_2, and d_1 are either equal to zero, if $I = 1/2$, as in the case of $^{13}C^{3+}$, or by a factor of $10^{-3} - 10^{-4}$ smaller than the magnetic-dipole ones. This is due to an additional factor $(\alpha Z)^2$ in the electric-quadrupole contributions compared to the magnetic-dipole ones in the equations for the hyperfine-structure corrections to the Breit – Rabi formula coefficients and small values of Q for low-Z ions.

As one can see from Table 3, the corrections ϵ_1, δ_1, δ_2, δ_3, and η_1 for Li-like ions are several times smaller as compared to the corresponding ones for the $1s$ state of the same H-like isotopes [21]. However, they provide more precise determinations of the coefficients in the Breit – Rabi formula.

For $B = 1 - 10\,T$, an estimate of the terms of the third and higher orders with respect to B in Eq. (54) indicates that the contributions from these terms are negligibly small as compared to both magnetic dipole and electrical quadrupole corrections. However, it is very important to take into account $\epsilon_2 B^2$ and $\eta_2 B^2$ if $Z = 6 - 32$. This is due to the fact that these terms are comparable with the other corrections to the Breit – Rabi formula considered and the less Z is, the more appreciable the contributions from $\epsilon_2 B^2$ and $\eta_2 B^2$ become. One can see that for Li-like ions these terms are $10 - 10^3$ times bigger as compared to the case of the $1s$ state of the same H-like isotopes [21]. In the second-order approximation (54) with respect to B, formulas (2), (11), (83), and (92) do not contain B to a power higher than two under the square root. This is due to the fact that $h_2(F) = h_2(F')$.

The Breit – Rabi formula for the $2s$ state contains $\Delta E_{\text{HFS}}^{(2s)}$, and the coefficients in the formula and the corrections to them calculated above include the value of μ/μ_N. The uncertainties of the nuclear magnetic moments indicated in Table 3, as a rule, do not include errors due to unknown chemical shifts which, in some cases, can contribute on the level of a few tenths percents. Thus, carrying out the experiments on the Zeeman splitting with the aforesaid accuracy could provide

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the most precise determination of both $\Delta E_{\mathrm{HFS}}^{(2s)}$ and μ/μ_N. The corrections to the Breit – Rabi formula evaluated in this paper will be important for this determination.

7 Acknowledgements

References

[1] N. Hermanspahn, H. Häffner, H.-J. Kluge, W. Quint, S. Stahl, J. Verdú, and G. Werth, Phys. Rev. Lett. **84**, 427 (2000).

[2] H. Häffner, T. Beier, N. Hermanspahn, H.-J. Kluge, W. Quint, S. Stahl, J. Verdú, and G. Werth, Phys. Rev. Lett. **85**, 5308 (2000).

[3] J. L. Verdú, S. Djekić, S. Stahl, T. Valenzuela, M. Vogel, G. Werth, T. Beier, H.-J. Kluge, and W. Quint, Phys. Rev. Lett. **92**, 093002 (2004).

[4] S. A. Blundell, K. T. Cheng, and J. Sapirstein, Phys. Rev. A **55**, 1857 (1997).

[5] H. Persson, S. Salomonson, P. Sunnergren, and I. Lindgren, Phys. Rev. A **56**, R2499 (1997).

[6] T. Beier, I. Lindgren, H. Persson, S. Salomonson, P. Sunnergren, H. Häffner, and N. Hermanspahn, Phys. Rev. A **62**, 032510 (2000).

[7] A. Czarnecki, K. Melnikov, and A. Yelkhovsky, Phys. Rev. A **63**, 012509 (2001).

[8] S. G. Karshenboim, in *The Hydrogen Atom*, edited by S. G. Karshenboim *et al.* (Springer, Berlin, 2001), p. 651.

[9] S. G. Karshenboim, V. G. Ivanov, and V. M. Shabaev, Can. J. Phys. **79**, 81 (2001); Zh. Eksp. Teor. Fiz. **120**, 546 (2001) [JETP **93**, 477 (2001)].

[10] V. M. Shabaev, Phys. Rev. A **64**, 052104 (2001).

[11] V. M. Shabaev and V. A. Yerokhin, Phys. Rev. Lett. **88**, 091801 (2002).

[12] A. P. Martynenko and R. N. Faustov, Zh. Eksp. Teor. Fiz. **120**, 539 (2001) [JETP **93**, 471 (2001)].

[13] D. A. Glazov and V. M. Shabaev, Phys. Lett. A **297**, 408 (2002).

[14] T. Beier, H. Häffner, N. Hermanspahn, S. G. Karshenboim, H.-J. Kluge, W. Quint, S. Stahl, J. Verdú, and G. Werth, Phys. Rev. Lett. **88**, 011603 (2002).

[15] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. Lett. **89**, 143001 (2002); Phys. Rev. A **69**, 052503 (2004).

[16] V. M. Shabaev, D. A. Glazov, M. B. Shabaeva, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. A **65**, 062104 (2002).

[17] A. V. Nefiodov, G. Plunien, and G. Soff, Phys. Rev. Lett. **89**, 081802 (2002).

[18] S. G. Karshenboim and V. G. Ivanov, Can. J. Phys. **80**, 1305 (2002).

[19] D. L. Moskovkin, N. S. Oreshkina, V. M. Shabaev, T. Beier, G. Plunien, W. Quint, and G. Soff, Phys. Rev. A **70**, 032105 (2004).

[20] K. Pachucki, A. Czarnecki, U. D. Jentschura, and V. A. Yerokhin, Phys. Rev. A **72**, 022108 (2005).

[21] D. L. Moskovkin and V. M. Shabaev, Phys. Rev. A **73**, 052506 (2006).

[22] U. D. Jentschura, A. Czarnecki, K. Pachucki, and V. A. Yerokhin, Int. J. Mass Spectrometry **251**, 102 (2006).

[23] P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **77**, 1 (2005).

[24] G. Werth, H. Häffner, N. Hermanspahn, H.-J. Kluge, W. Quint, and J. Verdú, in *The Hydrogen Atom*, edited by S. G. Karshenboim *et al.* (Springer, Berlin, 2001), p. 204.

[25] V. M. Shabaev, D. A. Glazov, N. S. Oreshkina, A. V. Volotka, G. Plunien, H.-J. Kluge, and W. Quint, Phys. Rev. Lett. **96**, 253002 (2006).

[26] R. A. Hegstrom, Phys. Rev. A **11**, 421 (1975).

[27] L. Veseth, Phys. Rev. A **22**, 803 (1980).

[28] E. Lindroth and A. Ynnerman, Phys. Rev. A **47**, 961 (1993).

[29] Z.-C. Yan, Phys. Rev. Lett. **86**, 5683 (2001); J. Phys. B **35**, 1885 (2002).

[30] P. Indelicato, E. Lindroth, T. Beier, J. Bieron, A. M. Costa, I. Lindgren, J. P. Marques, A.-M. Martensson-Pendrill, M. C. Martins, M. A. Ourdane, F. Parente, P. Patte, G. S. Rodrigues, S. Salomonson, and J. P. Santos, Hyperfine Interact. **132**, 349 (2001).

[31] V. M. Shabaev, D. A. Glazov, M. B. Shabaeva, I. I. Tupitsyn, V. A. Yerokhin, T. Beier, G. Plunien, and G. Soff, Nucl. Instrum. Methods Phys. Res. B **205**, 20 (2003).

[32] D. A. Glazov, V. M. Shabaev, I. I. Tupitsyn, A. V. Volotka, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. A **70**, 062104 (2004).

[33] D. A. Glazov, A. V. Volotka, V. M. Shabaev, I. I. Tupitsyn, and G. Plunien, Phys. Lett. A **357**, 330 (2006).

[34] V. M. Shabaev, O. V. Andreev, A. N. Artemyev, S. S. Baturin, A. A. Elizarov, Y. S. Kozhedub, N. S. Oreshkina, I. I. Tupitsyn, V. A. Yerokhin, and O. M. Zherebtsov, Int. J. Mass Spectrometry **251**, 109 (2006).

[35] D. L. Moskovkin, V. M. Shabaev, and W. Quint, Opt. Spectrosc., to be published; arXiv: 0710.5630, 2007 (http://xxx.lanl.gov).

[36] G. Breit and I. I. Rabi, Phys. Rev. **38**, 2082 (1931).

[37] H. Kopfermann, *Kernmomente, 2. Auflage* (Akademische Verlagsgesellschaft, Frankfurt am Main, 1956).

[38] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron Atoms* (Springer, Berlin, 1957).

[39] S. A. Zapryagaev, Opt. Spektrosk. **47**, 18 (1979) [Opt. Spectrosc. **47**, 9 (1979)].

[40] W. Quint, J. Dilling, S. Djekić, H. Häffner, N. Hermanspahn, H.-J. Kluge, G. Marx, R. Moore, D. Rodriguez, J. Schönfelder, G. Sikler, T. Valenzuela, J. Verdú, C. Weber, and G. Werth, Hyperfine Interact. **132**, 453 (2001).

[41] V. M. Shabaev, Izv. VUZ Fiz. **33**, 43 (1990) [Sov. Phys. J. **33**, 660 (1990)].

[42] V. M. Shabaev, Phys. Rep. **356**, 119 (2002).

[43] B. Sz.-Nagy, Comm. Mat. Helv. **19**, 347 (1946/47); T. Kato, Progr. Theor. Phys. **4**, 514 (1949); **5**, 95 (1950); **5**, 207 (1950).

[44] I. Angeli, At. Data Nucl. Data Tables **87**, 185 (2004).

[45] W. R. Johnson and G. Soff, At. Data Nucl. Data Tables **33**, 405 (1985).

[46] V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. Lett. **93**, 130405 (2004).

[47] W. R. Johnson and J. Sapirstein, Phys. Rev. Lett. **57**, 1126 (1986).

[48] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A. **37**, 307 (1988).

[49] M. B. Shabaeva and V. M. Shabaev, Phys. Rev. A. **52**, 2811 (1995).

[50] P. Raghavan, At. Data Nucl. Data Tables **42**, 189 (1989).

[51] P. Pyykkö, Mol. Phys. **99**, 1617 (2001).

Table 1: The numerical results for the extended-charge-nucleus values of functions $U_2^{(\mathrm{t})}(\alpha Z)$, $S_2^{(\mathrm{t})}(\alpha Z)$, and $T_2^{(\mathrm{t})}(\alpha Z)$ (for the ions with $I \neq 1/2$). The values of $\langle r^2 \rangle^{1/2}$ are taken from Ref. [44].

Ion	$^{13}\mathrm{C}^{3+}$	$^{17}\mathrm{O}^{5+}$	$^{21}\mathrm{Ne}^{7+}$	$^{25}\mathrm{Mg}^{9+}$	$^{33}\mathrm{S}^{13+}$	$^{43}\mathrm{Ca}^{17+}$	$^{53}\mathrm{Cr}^{21+}$
Z	6	8	10	12	16	20	24
$\langle r^2 \rangle^{1/2}$, fm	2.461	2.695	2.967	3.028	3.251	3.493	3.659
$U_2(\alpha Z)$	0.998574	0.997464	0.996038	0.994295	0.989858	0.984153	0.977179
$B_{\vec{B}}(\alpha Z)$	2.47400	2.47359	2.47305	2.47240	2.47070	2.46848	2.46568
$U_2^{(\mathrm{t})}(\alpha Z)$	1.41(14)	1.31(8)	1.24(5)	1.20(3)	1.144(19)	1.108(12)	1.080(9)
$S_2(\alpha Z)$	1.00306	1.00545	1.00854	1.01235	1.02218	1.03513	1.05145
$B_\mu(\alpha Z)$	-1.60040	-1.60757	-1.61684	-1.62825	-1.65769(1)	-1.69639(1)	-1.74505(2)
$S_2^{(\mathrm{t})}(\alpha Z)$	0.74(9)	0.80(5)	0.85(3)	0.88(2)	0.919(13)	0.950(8)	0.979(6)
$T_2(\alpha Z)$	———	1.00448(2)	1.00710(2)	1.01051(3)	1.01927(4)	1.03083(7)	1.04531(10)
$T_2^{(\mathrm{t})}(\alpha Z)$	———	1.0(3)	1.0(2)	1.01(17)	1.02(13)	1.03(10)	1.05(9)

Ion	$^{61}\mathrm{Ni}^{25+}$	$^{67}\mathrm{Zn}^{27+}$	$^{73}\mathrm{Ge}^{29+}$
Z	28	30	32
$\langle r^2 \rangle^{1/2}$, fm	3.822	3.964	4.063
$U_2(\alpha Z)$	0.968938	0.964342	0.959428
$B_{\vec{B}}(\alpha Z)$	2.46226	2.46030	2.45817
$U_2^{(\mathrm{t})}(\alpha Z)$	1.057(6)	1.046(5)	1.036(5)
$S_2(\alpha Z)$	1.07146(1)	1.08296(1)	1.09555(2)
$B_\mu(\alpha Z)$	-1.80458(3)	-1.83874(3)	-1.87609(4)
$S_2^{(\mathrm{t})}(\alpha Z)$	1.007(5)	1.022(4)	1.037(4)
$T_2(\alpha Z)$	1.06287(11)	1.07277(14)	1.08359(13)
$T_2^{(\mathrm{t})}(\alpha Z)$	1.06(8)	1.07(7)	1.08(7)

Table 2: The individual contributions to the ground-state g_j factor of lithiumlike ions with nonzero nuclear spin and the nuclear charge in the range $Z = 6 - 32$. The values of $\langle r^2 \rangle^{1/2}$ are the same as in Table 1.

Ion	$^{13}\mathrm{C}^{3+}$	$^{17}\mathrm{O}^{5+}$	$^{33}\mathrm{S}^{13+}$	$^{43}\mathrm{Ca}^{17+}$
g_D	1.999680300	1.999431380	1.997718193	1.996426011
Δg_int	0.000130758(19)	0.00017666(3)	0.00036124(9)	0.00045445(14)
Δg_QED	0.002319417(6)	0.002319549(12)	0.00232070(6)	0.00232171(10)
$\Delta g_\mathrm{rec}^{(e)}$	0.000000009	0.000000016	0.000000045(1)	0.000000057(2)
Δg_NS	0.0	0.0	0.000000005	0.000000014
g_j	2.00213048(2)	2.00192760(3)	2.00040018(11)	1.99920224(17)

Ion	$^{53}\mathrm{Cr}^{21+}$	$^{73}\mathrm{Ge}^{29+}$
g_D	1.994838064	1.990752307
Δg_int	0.0005485(2)	0.0007397(4)
Δg_QED	0.00232304(15)	0.0023270(2)
$\Delta g_\mathrm{rec}^{(e)}$	0.000000069(4)	0.000000093(9)
Δg_NS	0.000000035	0.000000160
g_j	1.9977097(3)	1.9938193(4)

Table 3: The numerical values of the coefficients in Eqs. (2), (9), (11), (83), (89), and (92) for Li-like ions with $Z = 6 - 32$. The values of μ/μ_N and Q are taken from Refs. [50] and [51], respectively.

Ion	^{13}C^{3+}	^{17}O^{5+}	^{33}S^{13+}	^{43}Ca^{17+}
I	1/2	5/2	3/2	7/2
μ/μ_N	0.7024118(14)	-1.89379(9)	0.6438212(14)	-1.317643(7)
Q, barn	——	-0.02558(22)	-0.0678(13)	-0.0408(8)
a_1	——	0.00041256(2)	-0.0002337573(5)	0.0002050317(11)
ϵ_1	——	-0.0000284(18)	-0.0000653(9)	-0.0000843(7)
$a_1(1+\epsilon_1)$	——	0.00041254(2)	-0.0002337421(6)	0.0002050144(11)
$\epsilon_2(=\eta_2)$	1.03(10)$\times10^4$	5.4(3)$\times10^3$	1.17(2)$\times10^3$	7.28(8)$\times10^2$
c_1	——	2.00151505(4)	2.00063394(11)	1.99899721(17)
δ_1	——	0.0000000059(4)	-0.00000000763(11)	0.00000000864(7)
$c_1(1+\delta_1)$	——	2.00151506(4)	2.00063393(11)	1.99899722(17)
c_2	4.01159069(8)	4.00606248(15)	4.0025362(4)	3.9959898(7)
δ_2	-0.0000000151(18)	0.0000000117(7)	-0.0000000152(2)	0.00000001730(15)
δ_3	——	0.0	-0.00000000001	0.0
$c_2(1+\delta_2)$	4.01159062(8)	4.00606253(15)	4.0025361(4)	3.9959899(7)
$c_2\delta_3$	——	0.0	-0.00000000002(1)	0.0
d_1	1.000682697(10)	1.00199519(5)	0.99984946(5)	1.00031873(9)
η_1	0.0000000075(9)	-0.0000000292(18)	0.0000000229(3)	-0.0000000605(5)
$d_1(1+\eta_1)$	1.000682704(10)	1.00199516(5)	0.99984948(5)	1.00031867(9)

| Ion	^{53}Cr^{21+}	^{73}Ge^{29+}
I	3/2	9/2
μ/μ_N	-0.47454(3)	-0.8794677(2)
Q, barn	-0.150(50)	-0.196
a_1	0.000172295(11)	0.00010643846(2)
ϵ_1	-0.0001041(6)	-0.0001472(6)
$a_1(1+\epsilon_1)$	0.000172277(11)	0.00010642279(7)
$\epsilon_2(=\eta_2)$	4.93(4)$\times10^2$	2.660(13)$\times10^2$
c_1	1.9975374(3)	1.9937129(4)
δ_1	0.00000000893(5)	0.00000000776(3)
$c_1(1+\delta_1)$	1.9975374(3)	1.9937129(4)
c_2	3.9901556(10)	3.9748910(17)
δ_2	0.00000001803(11)	0.00000001582(6)
δ_3	-0.00000000004(2)	-0.00000000001
$c_2(1+\delta_2)$	3.9901557(10)	3.9748911(17)
$c_2\delta_3$	-0.00000000018(6)	-0.00000000005
d_1	0.99911329(13)	0.9973886(2)
η_1	-0.00000002699(17)	-0.0000000708(3)
$d_1(1+\eta_1)$	0.99911326(13)	0.9973886(2)
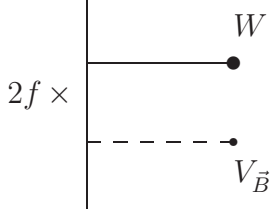
Figure 1: The second-order diagrams contributing to $S_2^{(t)}(\alpha Z)$, $T_2^{(t)}(\alpha Z)$ (if $f = 1$ and $W = V_{\text{HFS}}^{(\mu)}$ or $W = V_{\text{HFS}}^{(Q)}$), and $U_2^{(t)}(\alpha Z)$ (if $f = \frac{1}{2}$ and $W = V_{\vec{B}}^{(e)}$).
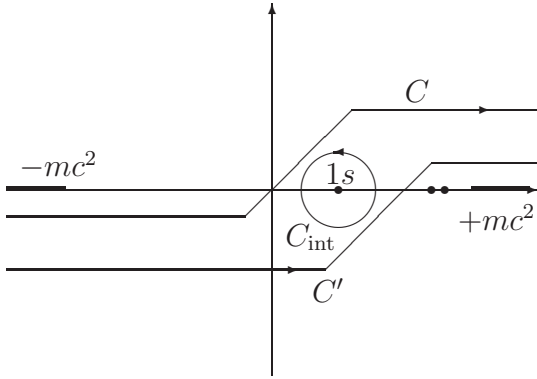

Figure 2: C is the original contour of the integration over the electron energy variable in the formalism with the standard vacuum. C' is the integration contour for the vacuum with the $(1s)^2$ shell included. The integral along the contour $C_{\text{int}} = C' - C$ describes the interaction of the valent electron with the $(1s)^2$-shell electrons.
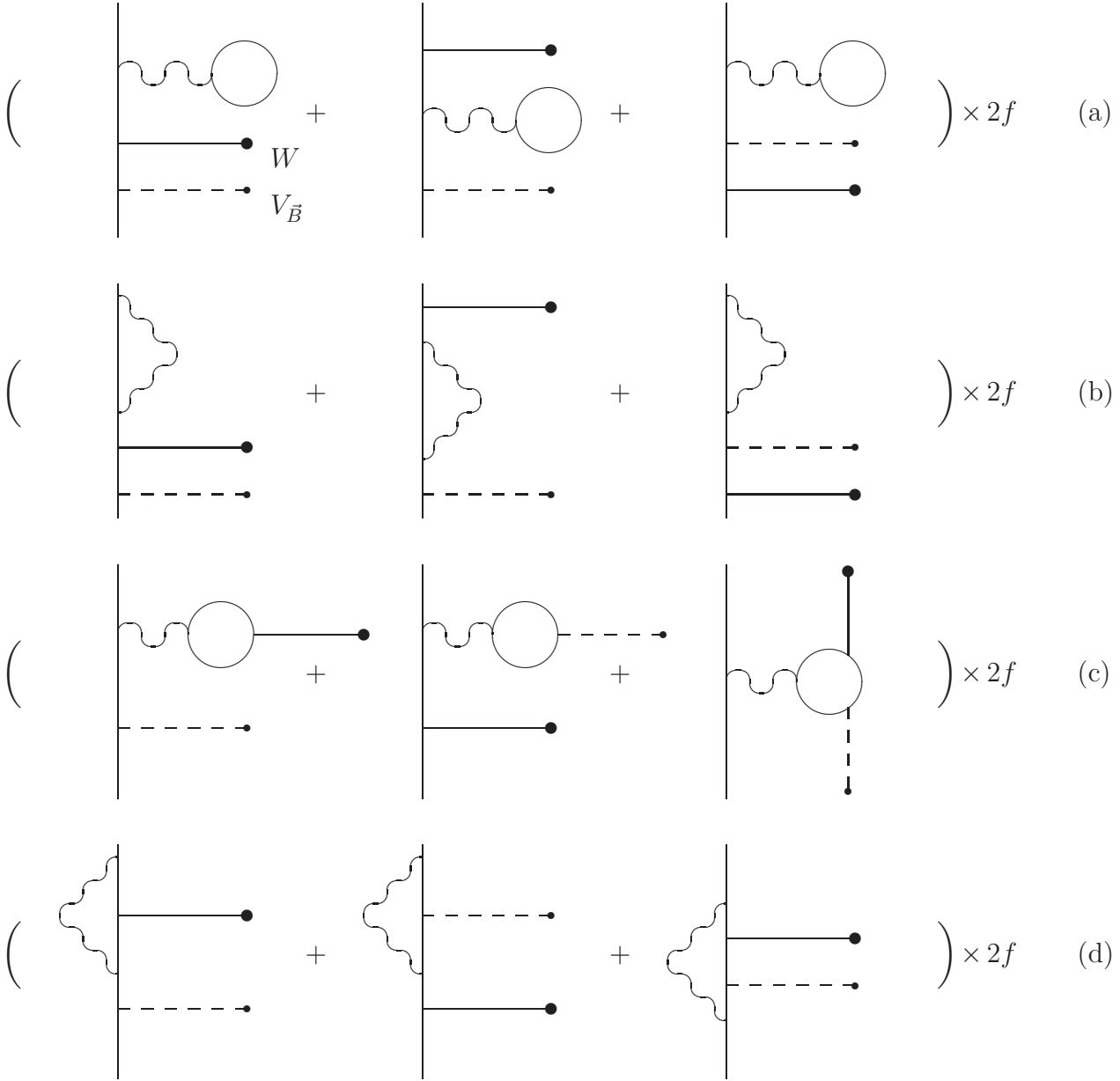
Figure 3: The third-order diagrams contributing to $S_2^{(t)}(\alpha Z)$ (if $f = 1$ and $W = V_{\mathrm{HFS}}^{(\mu)}$) and $U_2^{(t)}(\alpha Z)$ (if $f = \frac{1}{2}$ and $W = V_{\vec{B}}^{(e)}$) being combined with products of the lower-order diagrams presented in Figs. 4 and 5.
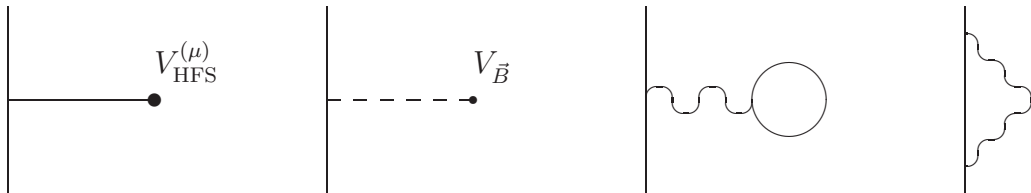

Figure 4: The first-order diagrams contributing to $S_2^{(t)}(\alpha Z)$ and $U_2^{(t)}(\alpha Z)$ being multiplied by the second-order diagrams presented in Fig. 5.
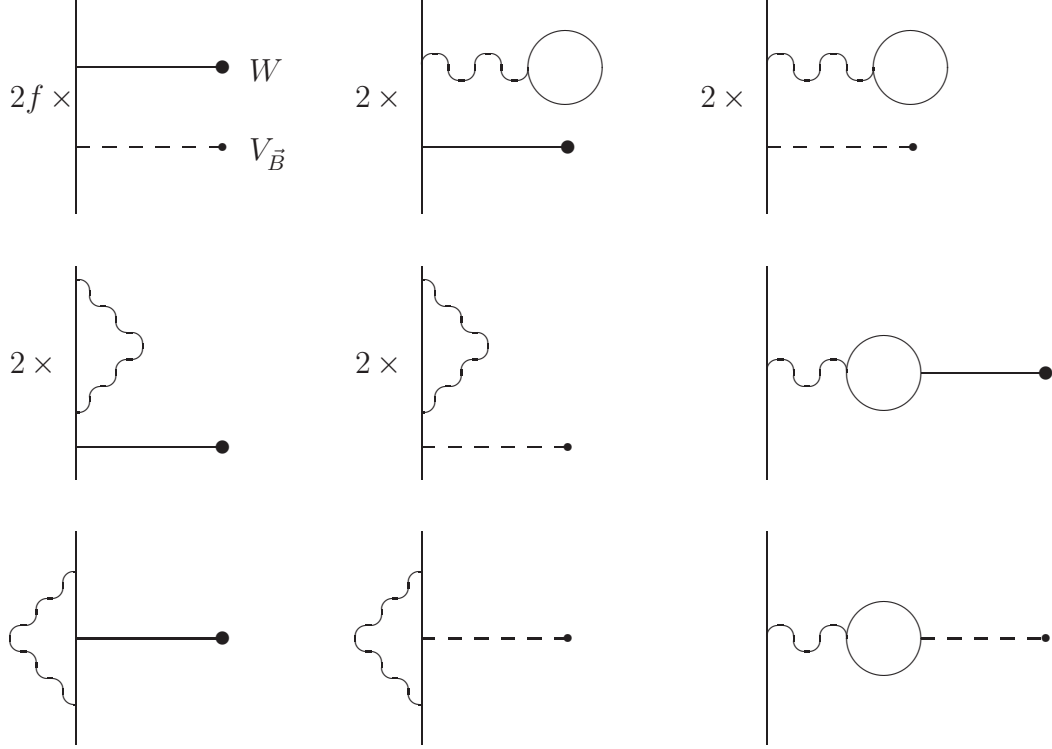
Figure 5: The second-order diagrams contributing to $S_2^{(\mathrm{t})}(\alpha Z)$ and $U_2^{(\mathrm{t})}(\alpha Z)$ being multiplied by the first-order diagrams presented in Fig. 4.